

Stability of nodal quasi-particles in superconductors with coexisting orders

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We establish a condition for the perturbative stability of zero energy nodal points in the quasi-particle spectrum of superconductors in the presence of coexisting *commensurate* orders. The nodes are found to be stable if the Hamiltonian is invariant under time reversal followed by a lattice translation. The principle is demonstrated with a few examples. Some experimental implications of various types of assumed order are discussed in the context of the cuprate superconductors.

One of the most distinct properties of unconventional (*e.g.* d-wave) superconductors is the possible existence of nodal quasi-particles (QP) with a linear Dirac-like spectrum in two dimensions, or lines of nodes in three dimensions. As the QP's dominate the low energy asymptotics of many physical properties, they are an essential feature of the state. A nodal QP spectrum in two dimensions has a linearly vanishing density of states at zero energy which produces several clear experimental fingerprints, *e.g.* a universal contribution to the thermal conductivity^{1,2}, a linear temperature dependence of the penetration depth at low temperatures³, and a \sqrt{H} dependence of the heat capacity in a magnetic field⁴. The spectrum can also be observed directly in ARPES and STM.

The cuprate high temperature superconductors are known to be d-wave superconductors, and the properties of their nodal QPs have been carefully explored in many experiments. Many theories have been proposed to account for the mechanism of superconductivity and the nature of the anomalous normal state. Some of these theories involve another type of ordering, that can either compete with superconductivity, coexist with it, or enhance it. Some examples, which we will treat explicitly, are antiferromagnetism, charge or spin density wave orders (*e.g.* “stripes”), and at least two forms of time-reversal symmetry breaking orbital antiferromagnetism: “d-density wave” (dDW) with an ordering vector $\mathbf{q} = (\pi, \pi)$ ⁵, and “Varma loops”⁶ which does not break the translational symmetry of the crystal, *i.e.* $\mathbf{q} = (0, 0)$, but at the same time has no net orbital moment. Various experimental and theoretical studies have provided evidence (sometimes conclusive, sometimes suggestive) of the existence of such “competing ordered states”⁷.

These observations lead us to address the following question: how is the quasi-particle spectrum of a d-wave superconductor generically affected by the presence of a coexisting order? Since the nodal QPs are gapless, it is not surprising that there exist (as we shall show) certain classes of infinitesimal perturbations that can change them qualitatively, either by gapping them, or by expanding the gapless locus in k-space from a point to a closed line (a “Fermi surface pocket”).

The question of the stability of the nodes was addressed in several previous studies, in particular in the presence of a general spin-orbit coupling⁸, in d-wave superconductor with several specific types of coexisting

order^{9,10,11,12,13,14,15} and in a vortex lattice^{16,17,18}.

In this paper, the question of the stability of the nodal QPs in the presence of a competing order of weak to moderate strength is addressed in the mean-field approximation. Specifically, we consider the quasi-particle spectrum of a 2d partially filled band in the presence of a uniform pairing field with d-wave symmetry and a second effective field, representing the competing order, which couples to a fermion bilinear and which we will consider as a “perturbation.” The competing order can break any symmetry, such as translation symmetry or time-reversal symmetry; the only condition is that it is *commensurate*, *i.e.* the period of the ordered state is a rational multiple of the original lattice constant. Under these assumptions, we show that if the perturbation does not “nest” any pair of nodes (*i.e.*, no two nodal k-points are coupled directly by the perturbation), and if the perturbation is invariant under time reversal or time reversal followed by a translation, then the nodes are stable at least until the strength of the perturbation exceeds a non-zero critical value. However, if the perturbation is not invariant under any such relative of time reversal symmetry, then the nodes can become gapped or can be shifted from zero energy for any infinitesimal amount of perturbation. (Even where the nodes are perturbatively stable, as the perturbation increases in strength, the location of the nodes in k-space generally shifts. In many cases, this eventually leads to a situation in which a pair of nodes meet or satisfy a more general nesting condition; then, they can annihilate each other leading to a gapped spectrum.)

We now turn to the derivation of our main result. Consider a two dimensional d-wave superconductor on a lattice, whose spectrum we assume is well approximated by a uniform BCS mean-field Hamiltonian, \mathcal{H}_0 . Suppose that we add a periodic perturbation with a fundamental ordering wave vector \mathbf{G} plus its harmonics. The period is assumed to be commensurate with the lattice, *i.e.* there exist integers N , n , and m such that $N\mathbf{G} = (\frac{2\pi n}{a}, \frac{2\pi m}{a})$. (It is straightforward to extend the proof to the case, such as a checkerboard CDW, in which there are two independent, commensurate ordering vectors, \mathbf{G}_1 and \mathbf{G}_2 , plus their combined harmonics.) The system is described by the effective Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{W} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger [h_0(\mathbf{k}) + w(\mathbf{k})] \Psi_{\mathbf{k}} \quad . \quad (1)$$

For each \mathbf{k} in the first Brillouin zone of the broken sym-

metry state, $h_0(\mathbf{k})$ and $w(\mathbf{k})$ are $2N \times 2N$ matrices, and $\Psi_{\mathbf{k}}^\dagger$ is the $2N$ component spinor operator,

$$\Psi_{\mathbf{k}}^\dagger = (\psi_{\mathbf{k}}^\dagger, \psi_{\mathbf{k}+\mathbf{G}}^\dagger, \psi_{\mathbf{k}+2\mathbf{G}}^\dagger, \dots), \quad (2)$$

$\psi_{\mathbf{k}}^\dagger = (c_{\mathbf{k}\uparrow}^\dagger, c_{-\mathbf{k}\downarrow}^\dagger)$ is the usual Nambu spinor, and $c_{\mathbf{k}\sigma}^\dagger$ creates an electron in the Bloch state of the non-interacting band with wave-vector \mathbf{k} and spin polarization σ .

Since \mathcal{H}_0 is the effective Hamiltonian of a uniform nodal superconductor, it is invariant under both time reversal, \mathcal{T} and translation, $\mathcal{S}_{\mathbf{R}}$, by any lattice vector \mathbf{R} , and hence it is invariant under the combined symmetry transformation, $\mathcal{T}_{\mathbf{R}} \equiv \mathcal{T}\mathcal{S}_{\mathbf{R}}$:

$$\mathcal{T}_{\mathbf{R}}^{-1} \mathcal{H}_0 \mathcal{T}_{\mathbf{R}} = \mathcal{H}_0. \quad (3)$$

Taking into account the fact that \mathcal{T} is anti-unitary, and so satisfies $\mathcal{T}^2 = -1$, it is straightforward to see that, with an appropriate choice of basis,

$$\mathcal{T}_{\mathbf{R}}^{-1} \Psi_{\mathbf{k}} \mathcal{T}_{\mathbf{R}} = \Lambda_{\mathbf{R}} \Psi_{\mathbf{k}}^* \quad (4)$$

where $\Lambda_{\mathbf{R}}$ is the tridiagonal unitary matrix

$$\Lambda_{\mathbf{R}} = \begin{pmatrix} i\sigma_2 e^{i\mathbf{k}\cdot\mathbf{R}} & & \\ & i\sigma_2 e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{R}} & \\ & & \ddots \end{pmatrix} \quad (5)$$

and σ_2 is a Pauli matrix. Moreover, by the usual arguments, it follows from the fermion anticommutation relations, Bloch's theorem, and Kramer's theorem that $h_0(\mathbf{k})$ is a real, traceless, block diagonal matrix. Specifically, in the neighborhood of a nodal point, \mathbf{k}_n ,

$$h_0 = \begin{pmatrix} h'_0 & 0 \\ 0 & h''_0 \end{pmatrix} \quad (6)$$

where $h'_0(\mathbf{k})$ is a real, traceless, 2×2 matrix which asymptotically has the Dirac form, $h'_0(\mathbf{k}) \sim (\mathbf{k} - \mathbf{k}_n) \cdot (\mathbf{v}_F \sigma_3 + \mathbf{v}_\Delta \sigma_1)$, and $h''_0(\mathbf{k})$ is a real, traceless $(2N-2) \times (2N-2)$ matrix. (\mathbf{v}_F and \mathbf{v}_Δ are, respectively, the Fermi velocity and the gap slope, and $\mathbf{v}_F \cdot \mathbf{v}_\Delta = 0$.)

Thus far, we have simply reproduced the usual calculation of the quasiparticle spectrum in an awkward basis with an artificially reduced first Brillouin zone obtained by treating \mathbf{G} as a reciprocal lattice vector, and correspondingly we were forced to consider N times as many bands. The meaning of the statement that \mathbf{G} does not nest the nodal points is that, for \mathbf{k} in the neighborhood of \mathbf{k}_n , all the eigenvalues of h''_0 have a magnitude larger than a non-zero, positive constant, Δ'' . The key point is that h'_0 is a real, traceless matrix, so its zeros have codimension 2, which means, generically, one can expect nodal points in 2D or nodal lines in 3D.

We now proceed to demonstrate that if the perturbation, in addition to not nesting the nodal points, is invariant under $\mathcal{T}_{\mathbf{R}}$ for some \mathbf{R} , *i.e.* $\mathcal{T}_{\mathbf{R}}^{-1} \mathcal{W} \mathcal{T}_{\mathbf{R}} = \mathcal{W}$, then the nodal point may move from \mathbf{k}_n to a nearby point, $\tilde{\mathbf{k}}_n$,

but it remains a nodal point. From the invariance of \mathcal{W} and Eq. (4), it follows that

$$\Lambda_{\mathbf{R}}^\dagger w(\mathbf{k}) \Lambda_{\mathbf{R}} = -w(\mathbf{k}) \quad (7)$$

which immediately implies that w is traceless. To make further progress, we express w and $\Lambda_{\mathbf{R}}$ in block form, in the same way as we treated h_0 :

$$w = \begin{pmatrix} w' & u^\dagger \\ u & w'' \end{pmatrix}, \quad \Lambda_{\mathbf{R}} = \begin{pmatrix} \Lambda'_{\mathbf{R}} & 0 \\ 0 & \Lambda''_{\mathbf{R}} \end{pmatrix} \quad (8)$$

where $w'(\mathbf{k})$ and $w''(\mathbf{k})$ are, respectively, a 2×2 and a $(2N-2) \times (2N-2)$ Hermitian matrix, $u(\mathbf{k})$ is a $(2N-2) \times 2$ matrix, and $\Lambda'_{\mathbf{R}} = i\sigma_2 e^{i\mathbf{k}\cdot\mathbf{R}}$. Since $h'_0(\mathbf{k}_n)$ is gapped, for a small enough perturbation, the matrix $h'_0 + w'$ has an inverse and hence the low energy states in the region of \mathbf{k} -space near \mathbf{k}_n can be found *asymptotically exactly* (*i.e.* neglecting errors that vanish in proportion to E/Δ'') by diagonalizing the effective 2×2 Hamiltonian

$$h'_{\text{eff}}(\mathbf{k}) \equiv h'_0 + w' - u^\dagger (h''_0 + w'')^{-1} u. \quad (9)$$

In particular, at a nodal point of the full Hamiltonian, $h_{\text{eff}}(\mathbf{k})$ must have a zero eigenvalue. It is straightforward to see from Eq. (7) that

$$[\Lambda'_{\mathbf{R}}]^\dagger h_{\text{eff}} \Lambda'_{\mathbf{R}} = \sigma_2 h_{\text{eff}} \sigma_2 = -h_{\text{eff}}. \quad (10)$$

This, combined with the condition that it be Hermitian, implies that h_{eff} is also a real, traceless matrix, $h_{\text{eff}}(\mathbf{k}) = a(\mathbf{k}) \sigma_1 + b(\mathbf{k}) \sigma_3$ where $a(\mathbf{k})$ and $b(\mathbf{k})$ are real functions.

The robustness of the node follows directly. The quasiparticle spectrum derived from $h_{\text{eff}}(\mathbf{k})$ is $E(\mathbf{k}) = \pm \sqrt{a^2(\mathbf{k}) + b^2(\mathbf{k})}$, which vanishes only when $a(\mathbf{k}) = b(\mathbf{k}) = 0$. Since we have two tuning parameters, k_x and k_y , a solution generically exists. More specifically, for \mathbf{k} near \mathbf{k}_n , $a(\mathbf{k}) = \mathbf{v}_\Delta \cdot (\mathbf{k} - \mathbf{k}_n) + \delta a$ and $b(\mathbf{k}) = \mathbf{v}_F \cdot (\mathbf{k} - \mathbf{k}_n) + \delta b$ where δa and δb are small so long as the perturbation is weak; the node simply moves a small distance in \mathbf{k} -space. The nodes must be stable for a finite range of strength of the perturbation, which concludes our proof. Conversely, for a perturbation that nests the nodal points, or for which no symmetry of the form of $\mathcal{T}_{\mathbf{R}}$ exists, our proof breaks down, which suggests, but does not prove, that the nodal structure is fundamentally altered by this sort of symmetry breaking. This argument is related to the Wigner-von Neumann theorem¹⁹.

Examples - To illustrate the above principle, we explicitly compute the QP spectrum of the mean-field Hamiltonian of a d-wave superconductor in the presence of various symmetry-breaking orders that have been considered in the context of the cuprate high temperature superconductors. To be explicit, we assume an underlying band-structure such that $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$. The parameters used are $t = 1$, $t' = -0.25$ and $\mu = -0.9$, representing a generic cuprate-like band structure. The gap function is taken to be

$$\Delta_{\mathbf{k}} = \Delta_0 (\cos k_x - \lambda \cos k_y) \quad (11)$$

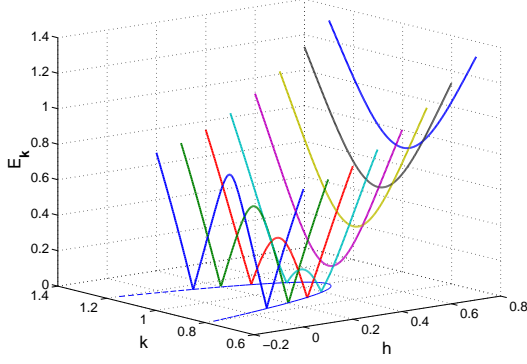


FIG. 1: (color online.) Spectrum of a d-wave superconductor along the line $(k_x, k_y) = (\frac{\pi}{2}, \frac{\pi}{2})k$ in the presence coexisting SDW order (*i.e.* a staggered Zeeman field) of magnitude h . The nodal points are stable until $h \approx 0.45$, when two nodal points meet in k -space and a gap opens.

with $\Delta_0 = 0.4$ and $\lambda = 1$. (In some cases, we will explore the effect of an orthorhombic distortion, which we will incorporate by letting $\lambda \neq 1$.)

As a first example, let us consider a $\mathbf{G} = (\pi, \pi)$ spin density wave, represented by the perturbation $\mathcal{W}_{\text{SDW}} = h \sum_{\mathbf{k}, \sigma} \sigma c_{\mathbf{k}+\mathbf{G}, \sigma}^\dagger c_{\mathbf{k}, \sigma}$. This perturbation manifestly breaks time reversal symmetry. However, it is invariant under time reversal followed by a translation by $\mathbf{R} = a\hat{\mathbf{x}}$. Diagonalizing the effective Hamiltonian numerically we find that the nodes in this case are robust. Upon increasing h , the nodes are shifted from their original position. Due to the reflection symmetry of the perturbation around the $\pi(1, 1)$ direction, the nodes are constrained to move along the $(0, 0)$ to $\pi(1, \pm 1)$ lines. When $h \approx 0.45$, the nodes reach the points $\pm \frac{\pi}{2}(1, 1)$, and so are nested by the ordering vector \mathbf{G} . For $h > 0.45$, the spectrum is fully gapped. The spectrum for various values of h is shown in Fig. 1 along the line $\mathbf{k} = \frac{\pi}{2}(k, k)$.

To illustrate further the special role played by translation symmetry, we will next consider the two combinations of spin and charge density waves (“stripes”), shown in Fig. 2 a & b. In both cases, time-reversal

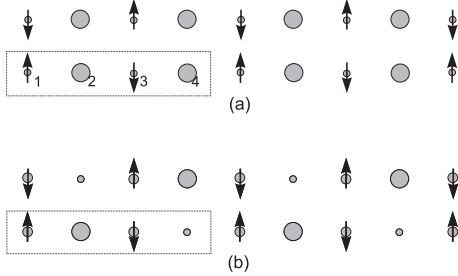


FIG. 2: Two patterns of unidirectional spin and charge order (“stripes”) discussed in the text. The arrows represent the spin density, and the size of the circles represents the charge density. The rectangles are the unit cells. The primitive vectors are $(4a, 0)$ and $(2a, a)$.

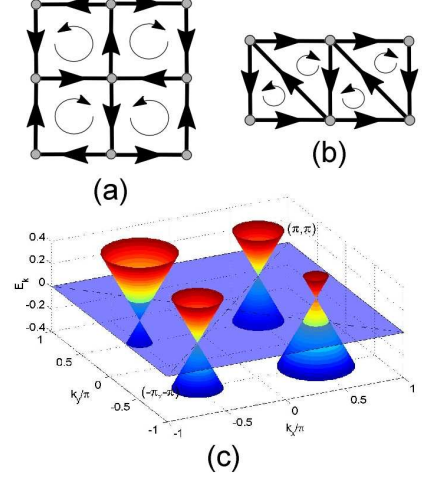


FIG. 3: (color online.) (a,b) Two patterns of spontaneous orbital currents on a square lattice. (a) the (π, π) d-density wave pattern, and (b) is a square lattice version of the $(0, 0)$ order proposed in 6. (c) Qualitative low energy spectrum of a d-wave superconductor with coexisting orbital current order of type (b). Note that the pair of nodes along the line $k_x = k_y$ remain at zero energy, while the nodes along $k_x = -k_y$ are shifted away from zero energy in opposite directions, forming hole-like or electron-like pockets.

and translation symmetry are broken, such that there are 4 sites in the new unit cell. However, in state-a, time reversal followed by translation by $\mathbf{R} = 2a\hat{\mathbf{x}}$, or by $\mathbf{R} = a\hat{\mathbf{y}}$, remains an unbroken symmetry, whereas in state-b, no symmetry of the form of $\mathcal{T}_{\mathbf{R}}$ survives. (There do, however, remain unbroken symmetries which combine \mathcal{T} and reflections through a plane.) We represent these states by a perturbation Hamiltonian of the form: $\mathcal{W} = \sum_{\mathbf{r}, \alpha} (V_{\alpha} n_{\mathbf{r}, \alpha} - h_{\alpha} S_{\mathbf{r}, \alpha}^z)$, where \mathbf{r} is the Bravais lattice vector labelling a unit cell, $\alpha = 1, \dots, 4$ is the index of the basis site in each unit cell, and $n_{\mathbf{r}, \alpha} = \sum_{\sigma} c_{\mathbf{r}, \alpha, \sigma}^\dagger c_{\mathbf{r}, \alpha, \sigma}$ and $S_{\mathbf{r}, \alpha}^z = \frac{1}{2} \sum_{\sigma} \sigma c_{\mathbf{r}, \alpha, \sigma}^\dagger c_{\mathbf{r}, \alpha, \sigma}$ are the local charge and spin densities, respectively. Following the site labelling scheme shown in Fig. 2, we take represent the effective field conjugate to the spin density by the 8 component vector $\mathbf{h} = (h, 0, -h, 0)$. In case a, the field conjugate to the density is $\mathbf{V} = (0, -V, 0, -V)$ while for case b, $\mathbf{V} = (0, -V, 0, V)$. We have computed the spectrum numerically for fixed h as a function of increasing V . As expected on the basis of our general theorem, in case-a the nodal points survive until V exceeds a critical value of order unity. Conversely, in case-b, where no general theorem insures the stability of the nodes, we find that a gap opens for arbitrarily small V and grows as $\Delta \sim V^2$.

The last example we will consider is the case of spontaneous orbital current loops. Fig. 3(a,b) shows two orbital current patterns: the first (a) is known as “d-density wave” (dDW)⁵ for which $\mathbf{G} = (\pi, \pi)$, and the second (b) is a $\mathbf{G} = (0, 0)$ pattern which, from a broken symmetry viewpoint, is equivalent to a state defined by Varma on the somewhat more complex Cu-O lattice in [6]. For

either of these states, the perturbation Hamiltonian is of the form $\mathcal{W} = -i \sum_{\mathbf{r}\mathbf{r}'} J_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} + H.c.$, where the connectivity of the current network $J_{\mathbf{r}\mathbf{r}'}$ is determined according to Fig. 3(a,b), and all the non-zero currents have the same magnitude J . Based on our general principle, we expect that in pattern (a) the superconducting nodes will survive at least over a finite range of J , since it is invariant under time reversal followed by a translation by $\mathbf{R} = a\hat{\mathbf{x}}$. Pattern (b), on the other hand, is a $\mathbf{G} = (0, 0)$ pattern, so the nodes may be removed immediately.

In fact, for pattern (a), $W_{\mathbf{k}} = 0$ at the nodal points (since it has d-wave symmetry), so the nodes are trivially stable. To avoid this non-generic situation, we introduce orthorhombicity of the gap function by setting $\lambda = 0.5$ in Eq. (11). Diagonalizing the BdG Hamiltonian numerically for this case, we still find that the nodes exist up to values of J of the order of the bandwidth t . Since pattern (b) does not break translation symmetry, the corresponding effective Hamiltonian can be easily diagonalized. The eigenenergies are $E_{\pm, \mathbf{k}}^{(b)} = \pm \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} + 2J \{\sin(k_x a) - \sin(k_y a) + \sin[(k_y - k_x) a]\}$. We see that even though the degeneracy at the nodes is not lifted, some of the nodes (the ones that lie on the line $k_x = -k_y$) are shifted away from zero energy: if $J > 0$, then the node at $k_x > 0$ ($k_x < 0$) is shifted to positive (negative) energy, respectively. The low-energy spectrum is shown qualitatively in Fig. 3(c). In the case of an orthorhombic gap function ($\lambda \neq 1$), the nodes along $k_x = k_y$ are also shifted to finite energies by an amount proportional to $\lambda - 1$. Whenever a node is shifted to a finite energy, a hole-like or electron-like pocket is formed, giving rise to a finite density of states at zero energy.

Discussion - The condition established here for the perturbative stability of the nodal points is a sufficient condition, not a necessary one. However, from the examples considered above, we see that in several cases where the condition is not met, the nodes are gapped or shifted to finite energies upon introducing an infinitesimal perturbation. Therefore, we expect that in generic cases, this condition is more or less necessary for the existence of nodal points. Thus, we can classify various weakly ordered states according to whether they leave the QP

nodes intact (*e.g.* dDW or certain types of stripes), gaps them (*e.g.* density wave order with ordering vector \mathbf{G} which nests the nodal points), or moves them away from the Fermi energy (*e.g.* Varma loops). Since the existence of nodal points has several well-defined experimental consequences, this information can provide a non-trivial consistency check on the assumed occurrence of various forms of coexisting order in the superconducting phase. In particular, in situations where the experiments are consistent with nodal QPs, one can rule out (or at least give an upper bound on) competing orders which are not invariant under time reversal followed by translation. For instance, measurements of the linear in T decay of the superfluid density in ultra-pure crystals of the Ortho-II phase of YBCO²⁰ give evidence that the nodal points are gapless and tied to the Fermi energy to within an accuracy of approximately 1K, or in other words a fraction of a percent of Δ_0 . This can probably be converted into a rather stringent bound on the strength of Varma loop order at low temperatures in this material.

The extension of these results to the case of an incommensurate perturbation is an interesting open problem.

A “striped superconducting” state²¹, which can be thought of as a spontaneously developed FFLO state, was considered as a candidate state to explain some extremely anomalous transport data²² that was recently obtained on the stripe-ordered material $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$. In the proposed state, the superconducting order parameter is modulated with wavevector $\mathbf{G} = (\pi/4, 0)$. A calculation of the spectrum in this state reveals that the nodes expand to a series of pockets along the bare Fermi surface, and the single particle spectral function has low energy weight along finite Fermi arcs. The reason that the nodes are not protected, despite the time reversal symmetry of this state, is that it cannot be viewed as a perturbed version of a uniform d-wave state.

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